

# **CHEMISTRY**

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### Supporting Information

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# Oxidative Rearrangements of Tricyclic Vinylcyclobutane Derivatives

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Geometries and energies of all stationary points calculated in the paper:

Compound 1

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1a - B3LYP/6-31G\*  
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0,1

6	-2.809211	-1.556665	0.694529
6	-1.949719	-0.702789	0.136008
6	-2.269149	0.331160	-0.926589
6	-1.422227	1.549743	-0.498864
6	-0.141259	0.981813	0.173163
6	-0.500421	-0.520361	0.503226
6	0.511682	-0.998458	-0.593706
6	0.927838	0.488176	-0.866274
6	1.769728	-1.727423	-0.094410
6	2.681912	-0.613625	0.456551
6	2.419723	0.579205	-0.486655
6	0.331654	1.879607	1.312743
1	-2.502654	-2.245932	1.478006
1	-3.851728	-1.603108	0.387873
1	-1.943071	-0.030138	-1.913273
1	-3.338870	0.550796	-1.004372
1	-1.189118	2.225943	-1.330325
1	-1.985365	2.130295	0.243132
1	-0.262876	-0.877626	1.511795
1	0.028195	-1.531003	-1.418718
1	0.749973	0.869181	-1.878565
1	2.262808	-2.222591	-0.941782
1	1.543253	-2.504039	0.646256
1	2.390626	-0.361943	1.484184
1	3.737739	-0.904920	0.487671
1	2.699009	1.543308	-0.046787
1	3.021456	0.459731	-1.397463
1	1.212723	1.482131	1.826615
1	0.586848	2.882791	0.946154
1	-0.462249	1.994824	2.061268

Electronic energy = -468.080565

Sum of electronic and zero-point Energies= -467.806915

Sum of electronic and thermal Enthalpies = -467.795343

Sum of electronic and thermal Free Energies= -467.842348

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1b - B3LYP/6-31G\*  
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0,1

6	2.500958	1.967510	0.296176
6	1.913559	0.771348	0.230043
6	2.586784	-0.538696	-0.140083
6	1.459170	-1.361340	-0.794465
6	0.176584	-0.996818	0.008728
6	0.443551	0.479392	0.459723
6	-0.594802	0.984448	-0.599928
6	-0.999438	-0.503291	-0.902875
6	-1.845176	1.675150	-0.037041
6	-2.673411	0.530222	0.579388
6	-2.447697	-0.648417	-0.390491
6	-0.121189	-2.029771	1.092385
1	1.945966	2.864290	0.562687
1	3.560378	2.098564	0.087776
1	3.465340	-0.407014	-0.781099
1	2.931300	-1.045685	0.774341
1	1.349937	-1.056412	-1.842886
1	1.659510	-2.439048	-0.791355
1	0.133358	0.712795	1.486397
1	-0.129732	1.541622	-1.418133
1	-0.912957	-0.841743	-1.941129
1	-2.409149	2.139845	-0.857260
1	-1.604455	2.467624	0.682292
1	-2.290628	0.282958	1.578216
1	-3.732264	0.785228	0.699117
1	-2.652261	-1.623765	0.065247
1	-3.131439	-0.549041	-1.243758
1	-0.931112	-1.710663	1.758235
1	-0.409622	-2.994276	0.654643
1	0.764476	-2.203710	1.717318

Electronic energy = -468.078341  
Sum of electronic and zero-point Energies= -467.804977  
Sum of electronic and thermal Enthalpies = -467.793345  
Sum of electronic and thermal Free Energies= -467.840637

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1c - B3LYP/6-31G\*  
-----

0,1

6	-2.879100	-1.627702	0.469297
6	-1.986122	-0.736859	0.034651
6	-2.208852	0.296305	-1.053592
6	-1.456551	1.534814	-0.521641
6	-0.226721	0.981212	0.240600
6	-0.607007	-0.510158	0.603607
6	0.572577	-1.018161	-0.287868
6	0.894329	0.443909	-0.731401
6	1.847302	-1.519908	0.421855
6	2.981862	-0.737832	-0.266505
6	2.397923	0.681287	-0.449601
6	0.200621	1.886668	1.389847
1	-2.652983	-2.313537	1.282642
1	-3.869403	-1.708888	0.026857

1	-1.755600	-0.045524	-1.996341
1	-3.268091	0.483023	-1.258097
1	-1.172139	2.240380	-1.311981
1	-2.106456	2.074112	0.180196
1	-0.532657	-0.805703	1.656107
1	0.267573	-1.703954	-1.086127
1	0.656485	0.660754	-1.778971
1	1.972258	-2.606605	0.358354
1	1.817201	-1.261975	1.489580
1	3.919174	-0.746522	0.302068
1	3.193829	-1.183459	-1.247832
1	2.548784	1.264047	0.465804
1	2.891127	1.233754	-1.256893
1	1.011793	1.453515	1.985196
1	0.541675	2.864876	1.025882
1	-0.644127	2.060269	2.068057

Electronic energy = -468.077227  
Sum of electronic and zero-point Energies= -467.803751  
Sum of electronic and thermal Enthalpies = -467.792049  
Sum of electronic and thermal Free Energies= -467.839740

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1d - B3LYP/6-31G\*  
-----

0,1

6	2.425379	2.078587	0.381511
6	1.900472	0.864333	0.206386
6	2.612607	-0.341257	-0.387024
6	1.473845	-1.212895	-0.953661
6	0.290718	-1.030313	0.041099
6	0.479727	0.447437	0.527349
6	-0.670510	0.891808	-0.446235
6	-1.036945	-0.613064	-0.673783
6	-1.920868	1.589833	0.138537
6	-3.068525	0.585347	-0.105999
6	-2.391578	-0.791015	0.043412
6	0.263345	-2.143616	1.084943
1	1.851613	2.893359	0.817542
1	3.449911	2.307031	0.096413
1	3.370331	-0.071561	-1.131033
1	3.134540	-0.887437	0.413427
1	1.192892	-0.843814	-1.948243
1	1.759715	-2.264596	-1.070435
1	0.214227	0.628238	1.576181
1	-0.280420	1.408122	-1.328017
1	-1.111234	-0.944081	-1.716950
1	-2.115300	2.565962	-0.319285
1	-1.796114	1.762678	1.215643
1	-3.917003	0.725070	0.574025
1	-3.450360	0.700232	-1.129554
1	-2.250910	-1.006660	1.110121
1	-2.988508	-1.611081	-0.370980
1	-0.461256	-1.948265	1.882928
1	0.005836	-3.107929	0.627858
1	1.246037	-2.256384	1.561146

Electronic energy = -468.074633  
Sum of electronic and zero-point Energies= -467.801372  
Sum of electronic and thermal Enthalpies = -467.789601  
Sum of electronic and thermal Free Energies= -467.837428

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1a\*+ - B3LYP/6-31G\*  
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1,2			
6	-2.618343	-1.756638	0.649271
6	-1.884715	-0.672036	0.202674
6	-2.336434	0.362499	-0.799864
6	-1.421509	1.582040	-0.529597
6	-0.132038	1.044601	0.165047
6	-0.548543	-0.367096	0.635556
6	0.497144	-0.968800	-0.687379
6	0.922763	0.494738	-0.878217
6	1.658269	-1.762690	-0.122251
6	2.615354	-0.704775	0.457063
6	2.412686	0.513191	-0.469841
6	0.393142	1.992879	1.240310
1	-2.193693	-2.482516	1.337289
1	-3.651226	-1.903079	0.345782
1	-2.203680	-0.038016	-1.816415
1	-3.403841	0.585788	-0.703493
1	-1.195341	2.148149	-1.437102
1	-1.926365	2.266845	0.160405
1	-0.170278	-0.802470	1.559966
1	-0.121384	-1.463099	-1.434369
1	0.752456	0.898035	-1.880458
1	2.119344	-2.258803	-0.992750
1	1.368259	-2.561100	0.568272
1	2.343641	-0.466346	1.492685
1	3.651822	-1.051041	0.473751
1	2.717212	1.459798	-0.016238
1	3.011190	0.385248	-1.379727
1	1.252833	1.587899	1.780751
1	0.695924	2.945155	0.791091
1	-0.393533	2.202069	1.973927

Electronic energy = -467.789082  
Sum of electronic and zero-point Energies= -467.518085  
Sum of electronic and thermal Enthalpies = -467.505882  
Sum of electronic and thermal Free Energies= -467.554691  
S\*\*2 = 0.7647

-----  
1c\*+ - B3LYP/6-31G\*  
-----

1,2			
6	-2.492901	-1.922859	0.670051
6	-1.846312	-0.790825	0.193634
6	-2.319471	0.095122	-0.930379
6	-1.506429	1.406964	-0.781176
6	-0.279813	1.104065	0.140112
6	-0.594379	-0.302898	0.701083
6	0.598883	-0.911896	-0.470977
6	0.964619	0.575780	-0.659952
6	1.773525	-1.673081	0.132915
6	2.965341	-0.736896	-0.195845

6	2.381367	0.683270	-0.048449
6	-0.043507	2.213864	1.163269
1	-2.046311	-2.545646	1.440198
1	-3.476036	-2.206723	0.304877
1	-2.136019	-0.409109	-1.891338
1	-3.403732	0.248054	-0.884499
1	-1.199472	1.814260	-1.748337
1	-2.130391	2.166585	-0.300378
1	-0.256124	-0.611070	1.689531
1	0.073655	-1.414085	-1.281918
1	0.958131	0.888354	-1.710624
1	1.865452	-2.678746	-0.287541
1	1.680792	-1.786452	1.219545
1	3.820242	-0.917655	0.461668
1	3.296776	-0.910152	-1.226000
1	2.340005	0.952298	1.011827
1	2.983507	1.445740	-0.549768
1	0.746876	1.972524	1.878856
1	0.236729	3.143183	0.654805
1	-0.959606	2.404986	1.733394

Electronic energy = -467.783224  
Sum of electronic and zero-point Energies= -467.512605  
Sum of electronic and thermal Enthalpies = -467.500032  
Sum of electronic and thermal Free Energies= -467.550468

S\*\*2 = 0.7636

-----  
1d\*+ - B3LYP/6-31G\*  
-----

1,2

6	2.334425	-2.065180	-0.668444
6	1.815625	-0.849951	-0.239833
6	2.514758	0.139198	0.654098
6	1.460259	1.227082	0.982061
6	0.307743	1.087759	-0.071407
6	0.528665	-0.339559	-0.619592
6	-0.677406	-0.817832	0.607699
6	-1.036460	0.679437	0.610738
6	-1.842466	-1.647424	0.081247
6	-3.015152	-0.631056	0.073367
6	-2.346938	0.732014	-0.203862
6	0.291703	2.224125	-1.092845
1	1.752952	-2.739380	-1.291171
1	3.341825	-2.374669	-0.403558
1	2.963205	-0.327931	1.538426
1	3.357154	0.554230	0.078605
1	1.075396	1.078842	1.996128
1	1.896829	2.228183	0.955671
1	0.097355	-0.649538	-1.571030
1	-0.135412	-1.217492	1.463572
1	-1.168043	1.100859	1.615472
1	-2.021174	-2.520752	0.717316
1	-1.657587	-2.032277	-0.928861
1	-3.780461	-0.888767	-0.663692
1	-3.495797	-0.622072	1.058166
1	-2.143327	0.831522	-1.276607
1	-2.975054	1.579965	0.081664
1	-0.439403	2.062663	-1.890210

1	0.046465	3.170124	-0.597575
1	1.276539	2.334809	-1.561687

Electronic energy = -467.783259  
Sum of electronic and zero-point Energies= -467.512986  
Sum of electronic and thermal Enthalpies = -467.500349  
Sum of electronic and thermal Free Energies= -467.550580  
S\*\*2 = 0.7637

-----  
4a\*+ - B3LYP/6-31G\*  
-----

1,2			
6	-2.878684	-1.335280	0.863415
6	-1.906615	-0.789082	0.081518
6	-2.164986	0.179803	-1.053793
6	-1.458215	1.482522	-0.597816
6	-0.138562	1.162900	0.079106
6	-0.520862	-0.957255	0.399250
6	0.586250	-0.965211	-0.643246
6	0.951619	0.567760	-0.790600
6	1.882622	-1.657339	-0.175258
6	2.688742	-0.560091	0.537390
6	2.416980	0.693579	-0.314024
6	0.148287	1.833516	1.376355
1	-2.635959	-1.949797	1.726038
1	-3.932148	-1.210919	0.629271
1	-1.744399	-0.190625	-1.996226
1	-3.230631	0.351875	-1.220716
1	-1.260346	2.150379	-1.448166
1	-2.106367	2.019934	0.100971
1	-0.276990	-1.352871	1.386033
1	0.203613	-1.379843	-1.582269
1	0.822029	0.914909	-1.821852
1	2.425705	-2.007343	-1.060325
1	1.682821	-2.534251	0.449768
1	2.326285	-0.423793	1.565045
1	3.753760	-0.797291	0.607219
1	2.621656	1.633112	0.207938
1	3.057752	0.682186	-1.202543
1	1.027300	1.445127	1.892521
1	0.345771	2.897625	1.150738
1	-0.719322	1.816657	2.042780

Electronic energy = -467.789613  
Sum of electronic and zero-point Energies= -467.518171  
Sum of electronic and thermal Enthalpies = -467.505745  
Sum of electronic and thermal Free Energies= -467.555238

S\*\*2 = 0.7634

-----  
4b\*+ - B3LYP/6-31G\*  
-----

1,2  
6 -3.086564 -1.309708 0.574619  
6 -1.973794 -0.795663 -0.030343  
6 -2.047731 0.225105 -1.146918  
6 -1.426710 1.524925 -0.566615  
6 -0.143361 1.226944 0.148558  
6 -0.677469 -1.095750 0.466883  
6 0.605411 -1.001058 -0.336020  
6 0.924458 0.520103 -0.643459  
6 1.868128 -1.525747 0.378197  
6 3.006320 -0.694523 -0.226255  
6 2.417616 0.729918 -0.280430  
6 0.109087 1.853086 1.466805  
1 -3.010222 -1.996617 1.412846  
1 -4.086248 -1.077802 0.219250  
1 -1.490262 -0.112569 -2.028312  
1 -3.075020 0.412383 -1.467540  
1 -1.202672 2.235966 -1.378126  
1 -2.138691 2.008009 0.108771  
1 -0.623315 -1.632176 1.414260  
1 0.469513 -1.534693 -1.288575  
1 0.754935 0.719097 -1.707310  
1 1.987800 -2.605153 0.241288  
1 1.797143 -1.338922 1.458141  
1 3.929430 -0.744572 0.357391  
1 3.238275 -1.048908 -1.237811  
1 2.529267 1.212094 0.695542  
1 2.914129 1.373586 -1.012020  
1 0.880050 1.349418 2.054200  
1 0.481610 2.877526 1.275330  
1 -0.808068 1.957543 2.052543

Electronic energy = -467.788573  
Sum of electronic and zero-point Energies= -467.517516  
Sum of electronic and thermal Enthalpies = -467.504870  
Sum of electronic and thermal Free Energies= -467.555315  
S\*\*2 = 0.7650

-----  
5b\*+ - B3LYP/6-31G\*  
-----

1,2  
6 -3.099692 -1.106700 0.602084  
6 -1.943634 -0.831192 -0.078491  
6 -0.712450 -1.435429 0.354303  
6 0.474650 -1.352754 -0.344299  
6 1.825178 -1.698707 0.181818  
6 2.882796 -0.655621 -0.254769  
6 2.474251 0.792831 0.127969  
6 -1.904860 0.188432 -1.188082  
6 -1.277819 1.574801 -0.747651  
6 -0.025588 1.457347 0.084345  
6 1.173996 1.151295 -0.515284  
6 -0.204761 1.655723 1.557547  
1 -3.117642 -1.816285 1.424815  
1 -4.045589 -0.649691 0.327106



1	-2.914395	0.388762	-1.556141
1	-1.331917	-0.192652	-2.039401
1	-1.077374	2.132233	-1.669415
1	-2.038089	2.126700	-0.187311
1	-0.706569	-1.921267	1.329535
1	0.428681	-1.107587	-1.402977
1	2.128190	-2.673291	-0.233508
1	1.800708	-1.808475	1.271690
1	3.846415	-0.898364	0.203217
1	3.024156	-0.717205	-1.341029
1	2.436558	0.895833	1.215736
1	3.259881	1.469576	-0.235713
1	1.185410	1.144049	-1.606811
1	-0.503548	2.697327	1.741289
1	-1.033881	1.038792	1.930492
1	0.686600	1.451382	2.151493

Electronic energy = -467.806767  
Sum of electronic and zero-point Energies= -467.535809  
Sum of electronic and thermal Enthalpies = -467.522859  
Sum of electronic and thermal Free Energies= -467.573327  
S\*\*2 = 0.7667

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TD-DFT calculation for 5b\*+  
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2.0716 eV 598.48 nm f=0.0843

45A -> 46A	-0.33610
43B -> 45B	0.11704
44B -> 45B	0.89257

2.9678 eV 417.77 nm f=0.0563

44A -> 46A	0.23873
45A -> 46A	-0.54097
43B -> 45B	0.77493
44B -> 45B	-0.18729
44B -> 46B	-0.14354
44B -> 47B	-0.11988

3.3369 eV 371.55 nm f=0.0877

45A -> 46A	0.70624
45A -> 47A	-0.14888
42B -> 45B	0.15980
43B -> 45B	0.55062
43B -> 48B	0.11182
44B -> 45B	0.10019
44B -> 46B	0.24895
44B -> 47B	0.14468

3.6360 eV 340.98 nm f=0.0053

45A -> 46A	-0.10701
42B -> 45B	0.97907

3.8418 eV 322.72 nm f=0.0148

44A -> 46A	-0.40062
44A -> 47A	0.19151
45A -> 46A	-0.10837
45A -> 47A	0.60775
38B -> 45B	0.11132
41B -> 45B	0.17991

43B -> 45B	0.10688
44B -> 46B	0.65806
44B -> 47B	-0.30800

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5c\*+ - B3LYP/6-31G\*  
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1,2			
6	3.058086	1.019972	0.718702
6	1.962429	0.781347	-0.025764
6	0.718881	1.538644	0.203083
6	-0.359373	1.488663	-0.596075
6	-1.767810	1.855175	-0.219110
6	-2.477065	0.668760	0.497719
6	-2.522737	-0.699634	-0.239551
6	1.944357	-0.354759	-1.038967
6	1.267361	-1.687014	-0.566013
6	-0.113938	-1.533117	0.058519
6	-1.177902	-1.233380	-0.701883
6	-0.155193	-1.587299	1.564249
1	3.074124	1.801434	1.474828
1	3.971071	0.443176	0.596679
1	2.976193	-0.597170	-1.319242
1	1.452221	-0.024938	-1.961266
1	1.217917	-2.346272	-1.442875
1	1.940521	-2.171300	0.152289
1	0.657451	2.081427	1.148340
1	-0.265864	0.983685	-1.551752
1	-2.340437	2.145493	-1.110132
1	-1.783520	2.712701	0.466641
1	-1.977694	0.530104	1.463343
1	-3.510599	0.967861	0.721534
1	-3.018217	-1.412127	0.435787
1	-3.183130	-0.612702	-1.111763
1	-1.027814	-1.232061	-1.783227
1	-1.174444	-1.584115	1.960247
1	0.345536	-2.494232	1.929021
1	0.384110	-0.735112	2.002090

Electronic energy = -467.793407  
Sum of electronic and zero-point Energies= -467.522745  
Sum of electronic and thermal Enthalpies = -467.509441  
Sum of electronic and thermal Free Energies= -467.561707  
S\*\*2 = 0.7613

-----  
TD-DFT calculation for 5c\*+  
-----

1.5908 eV 779.39 nm f=0.0887  
45A -> 46A -0.15956  
44B -> 45B 0.86905

2.5392 eV 488.28 nm f=0.0266  
44A -> 46A 0.14326  
45A -> 46A -0.20541  
41B -> 45B 0.11211  
42B -> 45B 0.12230  
43B -> 45B 0.94922

2.9772 eV 416.45 nm f=0.0101

44A -> 46A	-0.10567
45A -> 46A	0.18282
41B -> 45B	0.38639
42B -> 45B	0.89340
43B -> 45B	-0.10417

3.1561 eV 392.84 nm f=0.0095

45A -> 46A	0.13339
41B -> 45B	0.88526
42B -> 45B	-0.41755

3.4866 eV 355.61 nm f=0.0028

38B -> 45B	-0.17901
39B -> 45B	-0.22615
40B -> 45B	0.94782

3.6658 eV 338.22 nm f=0.0680

44A -> 46A	-0.25596
45A -> 46A	0.73790
36B -> 45B	0.10835
38B -> 45B	0.20017
41B -> 45B	-0.16936
43B -> 45B	0.17268
43B -> 48B	0.15588
44B -> 46B	0.57224

3.7855 eV 327.52 nm f=0.0203

45A -> 46A	-0.14886
38B -> 45B	0.71991
39B -> 45B	0.58824
40B -> 45B	0.27461
44B -> 46B	-0.10585

3.9474 eV 314.09 nm f=0.0113

45A -> 46A	0.12089
45A -> 47A	0.13795
36B -> 45B	0.16727
38B -> 45B	-0.59281
39B -> 45B	0.73509
44B -> 47B	-0.14361

-----  
6\*+ - B3LYP/6-31G\*  
-----

1,2

6	2.815290	-1.567384	-0.273875
6	1.888818	-0.612040	0.131142
6	2.235246	0.827743	0.346176
6	1.081580	1.754755	-0.141106
6	0.512174	-0.963493	0.346550
6	-0.287836	1.050218	-0.127403
6	-0.264255	-0.169599	-1.057916
6	-0.374335	0.053815	1.090727
6	-1.574704	-0.908316	-1.248834
6	-2.265111	-1.323817	0.075789
6	-1.786626	-0.500182	1.300440
6	-1.415662	2.068824	-0.330418
1	2.526595	-2.603298	-0.429957
1	3.860353	-1.311076	-0.422346

1	2.354911	0.962960	1.432435
1	3.193926	1.090177	-0.108408
1	1.046188	2.645186	0.493640
1	1.297575	2.099213	-1.159311
1	0.284131	-2.029019	0.383166
1	0.370714	-0.145669	-1.946214
1	-2.209447	-0.208715	-1.817131
1	-1.425554	-1.775566	-1.899444
1	-3.351411	-1.256954	-0.027738
1	-2.051368	-2.383589	0.251131
1	-2.464260	0.332359	1.511460
1	-1.797959	-1.138034	2.191488
1	0.061699	0.435216	2.023403
1	-2.403376	1.606217	-0.387344
1	-1.425520	2.783770	0.499153
1	-1.254680	2.633670	-1.255618

Electronic energy = -467.789561  
Sum of electronic and zero-point Energies= -467.517311  
Sum of electronic and thermal Enthalpies = -467.505395  
Sum of electronic and thermal Free Energies= -467.553169  
S\*\*2 = 0.7629

-----  
TS 1a\*+ --> 4a\*+ - B3LYP/6-31G\*  
-----

1,2			
6	-2.832648	-1.517599	0.751916
6	-1.940009	-0.687524	0.110824
6	-2.281105	0.336713	-0.945661
6	-1.381405	1.537953	-0.573874
6	-0.106590	0.998000	0.142045
6	-0.543818	-0.607439	0.449250
6	0.545377	-0.849713	-0.734866
6	1.037238	0.615925	-0.818972
6	1.726323	-1.696031	-0.246254
6	2.648412	-0.709122	0.489036
6	2.490566	0.607727	-0.300244
6	0.233524	1.716358	1.439898
1	-2.519105	-2.157345	1.572413
1	-3.874753	-1.572187	0.448964
1	-2.041283	-0.062638	-1.942450
1	-3.343976	0.591240	-0.958871
1	-1.113111	2.147975	-1.441188
1	-1.918477	2.185118	0.128067
1	-0.239842	-1.057357	1.394446
1	0.012812	-1.225427	-1.612082
1	0.947325	1.093521	-1.796728
1	2.218236	-2.070514	-1.156732
1	1.430183	-2.568347	0.344287
1	2.323418	-0.589569	1.530443
1	3.684000	-1.058444	0.523762
1	2.744148	1.496130	0.285756
1	3.160265	0.602812	-1.167268
1	1.080091	1.277539	1.971789
1	0.503961	2.751786	1.184440
1	-0.629082	1.744225	2.112356

Electronic energy = -467.785775  
 Sum of electronic and zero-point Energies= -467.515778  
 Sum of electronic and thermal Enthalpies = -467.503969  
 Sum of electronic and thermal Free Energies= -467.551988  
 S\*\*2 = 0.7633

Low frequencies --- -264.0155 -20.6026 -19.5385 -12.5631 0.0005 0.0007  
 Low frequencies --- 0.0007 67.1085 160.1136

-----  
 TS 4a\*+ --> 4b\*+ - B3LYP/6-31G\*  
 -----

1,2  
 6 -3.182647 -1.193046 0.542088  
 6 -2.052511 -0.676568 -0.042424  
 6 -2.120493 0.548623 -0.930265  
 6 -1.310653 1.675836 -0.240158  
 6 0.032881 1.201467 0.196825  
 6 -0.792794 -1.241534 0.260049  
 6 0.512096 -1.075172 -0.489430  
 6 0.840906 0.431952 -0.801913  
 6 1.742880 -1.625835 0.297411  
 6 2.874753 -0.571505 0.216572  
 6 2.381091 0.537235 -0.738519  
 6 0.577955 1.675973 1.486602  
 1 -3.137156 -2.058402 1.197051  
 1 -4.165664 -0.773523 0.350970  
 1 -1.717962 0.332160 -1.926091  
 1 -3.151322 0.881349 -1.072679  
 1 -1.147015 2.504132 -0.951958  
 1 -1.870918 2.086712 0.605507  
 1 -0.798957 -2.038417 1.003059  
 1 0.431183 -1.616415 -1.446649  
 1 0.473767 0.690900 -1.800601  
 1 2.047358 -2.582727 -0.135528  
 1 1.474437 -1.829261 1.338922  
 1 3.094363 -0.168505 1.210456  
 1 3.810026 -1.006634 -0.145461  
 1 2.725711 1.536035 -0.451570  
 1 2.756627 0.361199 -1.752001  
 1 1.458653 1.130123 1.825942  
 1 0.884484 2.729713 1.341425  
 1 -0.188394 1.697002 2.268180

Electronic energy = -467.784459  
 Sum of electronic and zero-point Energies= -467.513787  
 Sum of electronic and thermal Enthalpies = -467.501724  
 Sum of electronic and thermal Free Energies= -467.550692  
 S\*\*2 = 0.7669

Low frequencies --- -98.1616 -13.4438 -11.8531 -0.0010 -0.0008 -0.0003  
 Low frequencies --- 10.6865 82.1817 102.9059

-----  
TS 4b\*+ --> 5b\*+ - B3LYP/6-31G\*  
-----

1,2  
6 -3.185266 -1.228274 0.480448  
6 -2.001386 -0.775732 -0.069533  
6 -0.754586 -1.293428 0.314148  
6 0.557279 -0.981783 -0.356661  
6 1.804203 -1.517052 0.359382  
6 2.981526 -0.734411 -0.224015  
6 2.472151 0.720044 -0.264032  
6 -2.013386 0.357914 -1.076649  
6 -1.331952 1.644837 -0.483133  
6 -0.035032 1.305376 0.153931  
6 0.972894 0.632998 -0.636454  
6 0.132779 1.605630 1.587409  
1 -3.195842 -2.040390 1.201038  
1 -4.143898 -0.807342 0.195728  
1 -3.031690 0.634425 -1.359229  
1 -1.491770 0.068558 -1.995773  
1 -1.141426 2.342260 -1.311734  
1 -2.003521 2.125683 0.232228  
1 -0.724792 -2.068689 1.076169  
1 0.535890 -1.358407 -1.390218  
1 1.879554 -2.599722 0.203618  
1 1.720477 -1.352152 1.441243  
1 3.896841 -0.833734 0.365326  
1 3.205350 -1.086748 -1.237874  
1 2.610532 1.193263 0.712679  
1 3.001045 1.339743 -0.993832  
1 0.799814 0.799691 -1.701568  
1 0.309146 2.696316 1.651721  
1 -0.796855 1.425323 2.138056  
1 0.975807 1.105210 2.063369

Electronic energy = -467.786006  
Sum of electronic and zero-point Energies= -467.516935  
Sum of electronic and thermal Enthalpies = -467.504534  
Sum of electronic and thermal Free Energies= -467.554315  
S\*\*2 = 0.7797

Low frequencies --- -429.7514 -19.5178 -7.5196 -0.0013 -0.0009 -0.0008  
Low frequencies --- 5.3347 54.9748 98.3015

-----  
TS 5b\*+ --> 5c\*+ - B3LYP/6-31G\*  
-----

1,2  
6 -3.091750 -1.103406 0.683392  
6 -1.977310 -0.794600 -0.050466  
6 -0.731759 -1.438432 0.260388  
6 0.421638 -1.302000 -0.490108  
6 1.769176 -1.788426 -0.076583  
6 2.868035 -0.686883 0.172922  
6 2.508728 0.823297 -0.109649  
6 -1.995802 0.290302 -1.095747  
6 -1.309648 1.628074 -0.609721  
6 0.013602 1.437486 0.088224  
6 1.135859 1.106944 -0.636741

6	-0.003904	1.582478	1.577637
1	-3.066465	-1.862398	1.460535
1	-4.047357	-0.621886	0.498548
1	-3.023854	0.532200	-1.377333
1	-1.492999	-0.046579	-2.007942
1	-1.184267	2.256544	-1.498746
1	-2.004131	2.142565	0.060799
1	-0.681004	-2.016272	1.182490
1	0.318888	-0.983138	-1.523173
1	2.132984	-2.451955	-0.871920
1	1.671572	-2.395792	0.828576
1	3.174437	-0.764132	1.219051
1	3.750060	-0.946584	-0.416232
1	2.669875	1.385972	0.814290
1	3.228288	1.212240	-0.837082
1	1.033653	1.117524	-1.722359
1	-0.245308	2.622594	1.837991
1	-0.811164	0.973224	2.007041
1	0.935607	1.316861	2.064176

Electronic energy = -467.792640  
 Sum of electronic and zero-point Energies= -467.521338  
 Sum of electronic and thermal Energies= -467.509809  
 Sum of electronic and thermal Enthalpies = -467.508865  
 Sum of electronic and thermal Free Energies= -467.558912  
 S\*\*2 = 0.7677

Low frequencies --- -216.4458 -16.0186 -9.4575 -0.0006 -0.0006 -0.0005  
 Low frequencies --- 3.6288 45.0588 101.4694

Compound 2  
 \*\*\*\*\*

-----  
 2a - B3LYP/6-31G\*  
 -----

0,1

6	-0.977033	0.109409	-1.188050
6	0.581580	0.180726	-0.990064
6	0.544316	-1.122959	-0.122745
6	-1.020492	-1.184284	-0.303195
6	1.242270	1.251934	-0.147941
6	1.133313	-0.730211	1.261483
6	1.224615	2.569448	-0.364322
6	1.956926	0.551124	0.996115
6	-1.957524	-0.864007	0.875831
6	-1.889223	1.142096	-0.505764
6	-2.005780	0.676820	0.959995
1	1.110983	0.064539	-1.944819
1	-1.241972	-0.030048	-2.240461
1	-1.329955	-2.098920	-0.820476
1	1.732078	3.264767	0.300795
1	0.714384	3.004639	-1.220023
1	2.969260	0.272801	0.665207
1	2.078638	1.186237	1.880586
1	1.747050	-1.532499	1.686745
1	0.346755	-0.520258	1.991987
1	-2.877114	1.111692	-0.984568
1	-1.517627	2.168575	-0.588647
1	-2.959551	-1.246060	0.639454

1	-1.655364	-1.338536	1.817210
1	-2.915295	1.043254	1.449455
1	-1.155617	1.061061	1.535451
6	1.265787	-2.327875	-0.725344
1	2.351727	-2.167778	-0.753484
1	1.077233	-3.236028	-0.137867
1	0.931860	-2.520756	-1.752535

Electronic energy = -468.074491  
Sum of electronic and zero-point Energies= -467.800709  
Sum of electronic and thermal Enthalpies = -467.789242  
Sum of electronic and thermal Free Energies= -467.835946

-----  
2a\*+ - B3LYP/6-31G\*  
-----

1,2			
6	0.734614	-0.549924	-1.239110
6	-0.920386	0.186452	-0.885120
6	-0.124570	1.232776	-0.095047
6	1.302041	0.688565	-0.560651
6	-1.726158	-0.625507	-0.022442
6	-0.538664	0.975360	1.389102
6	-2.652298	-1.540756	-0.475320
6	-1.432808	-0.297096	1.422820
6	2.314054	0.165852	0.473853
6	1.215210	-1.787015	-0.509154
6	1.884448	-1.284920	0.792203
1	-1.276715	0.394571	-1.894022
1	0.671257	-0.614143	-2.325354
1	1.739232	1.406211	-1.260469
1	-3.292066	-2.088375	0.211377
1	-2.785434	-1.733247	-1.536424
1	-2.367926	-0.138261	1.972298
1	-0.944631	-1.148048	1.913882
1	-1.111111	1.839299	1.739561
1	0.321543	0.887191	2.054852
1	1.972305	-2.229119	-1.176437
1	0.455338	-2.561489	-0.368725
1	3.303284	0.165859	0.000657
1	2.390221	0.800338	1.361617
1	2.733651	-1.911853	1.075548
1	1.182375	-1.312926	1.629634
6	-0.350850	2.683044	-0.536500
1	-1.388360	2.985560	-0.355669
1	0.304667	3.353033	0.030917
1	-0.135423	2.824417	-1.601054

Electronic energy = -467.781481  
Sum of electronic and zero-point Energies= -467.510842  
Sum of electronic and thermal Enthalpies = -467.498392  
Sum of electronic and thermal Free Energies= -467.548066  
S\*\*2 = 0.7674



-----  
7a\*+ - B3LYP/6-31G\*  
-----

1,2  
6 0.675569 -0.481024 -1.226928  
6 -0.842197 -0.369364 -1.096402  
6 -0.135046 1.285846 0.073219  
6 1.173587 0.857179 -0.563405  
6 -1.690385 -0.822987 -0.032400  
6 -0.561015 0.771469 1.439938  
6 -2.977466 -1.184136 -0.292154  
6 -1.123025 -0.678786 1.362634  
6 2.378461 0.476751 0.325681  
6 1.435964 -1.636277 -0.510335  
6 2.212295 -1.014962 0.675361  
1 -1.358197 -0.111818 -2.021606  
1 0.904509 -0.473300 -2.295375  
1 1.451173 1.593965 -1.321480  
1 -3.644021 -1.513204 0.500051  
1 -3.373885 -1.196951 -1.303723  
1 -1.891210 -0.829834 2.124838  
1 -0.342187 -1.419101 1.548658  
1 -1.338052 1.435263 1.829966  
1 0.290830 0.825302 2.128303  
1 2.136447 -2.060247 -1.237070  
1 0.773809 -2.452974 -0.208027  
1 3.280395 0.626226 -0.277931  
1 2.481447 1.120309 1.205845  
1 3.180200 -1.502894 0.821911  
1 1.667401 -1.134270 1.616413  
6 -0.784810 2.535043 -0.417232  
1 -1.860090 2.555606 -0.217232  
1 -0.338769 3.370635 0.153327  
1 -0.591390 2.734764 -1.474727

Electronic energy = -467.781008  
Sum of electronic and zero-point Energies= -467.508817  
Sum of electronic and thermal Enthalpies = -467.496366  
Sum of electronic and thermal Free Energies= -467.545833  
S\*\*2 = 0.7633

-----  
7b\*+ - B3LYP/6-31G\*  
-----

1,2  
6 0.552114 -0.886031 -0.931579  
6 -0.948354 -1.028816 -1.002946  
6 0.129663 1.556473 -0.148023  
6 1.123324 0.506632 -0.460724  
6 -1.876319 -0.732567 0.003848  
6 -0.941034 1.420329 0.863802  
6 -3.205927 -1.076665 -0.142830  
6 -1.416322 0.012607 1.240715  
6 2.069004 0.186998 0.765094  
6 1.273214 -1.952505 -0.044561  
6 2.542814 -1.242939 0.446243  
1 -1.328618 -1.547395 -1.880685  
1 0.922148 -0.996604 -1.955455  
1 1.767154 0.884329 -1.260635  
1 -3.944114 -0.840763 0.617038

1	-3.555084	-1.614555	-1.019164
1	-2.234948	0.107903	1.958878
1	-0.620485	-0.539640	1.751547
1	-1.791620	2.043806	0.550065
1	-0.545716	1.954063	1.753050
1	1.478987	-2.865511	-0.610529
1	0.641022	-2.235371	0.804406
1	2.877850	0.918243	0.844082
1	1.509759	0.200697	1.705959
1	3.300799	-1.217047	-0.345684
1	2.995949	-1.723618	1.318934
6	0.288280	2.878829	-0.790877
1	-0.274934	3.677031	-0.301362
1	1.346435	3.151125	-0.892845
1	-0.087337	2.789237	-1.826569

Electronic energy = -467.785200  
Sum of electronic and zero-point Energies= -467.514902  
Sum of electronic and thermal Enthalpies = -467.502082  
Sum of electronic and thermal Free Energies= -467.553192  
S\*\*2 = 0.7720

-----  
8b\*+ - B3LYP/6-31G\*  
-----

1,2

6	0.578089	-1.434724	-0.998112
6	-0.792017	-1.278731	-0.932411
6	-0.123519	1.588560	-0.145363
6	1.207770	1.322687	-0.357059
6	-1.652666	-0.955609	0.184000
6	-0.836761	1.283640	1.143914
6	-2.991692	-1.191547	0.040863
6	-1.130980	-0.246585	1.405676
6	2.185925	0.743269	0.606229
6	1.595599	-1.691106	0.063639
6	2.720451	-0.628418	0.130443
1	-1.312564	-1.397369	-1.882169
1	0.972818	-1.530827	-2.010350
1	1.612750	1.583484	-1.335203
1	-3.697567	-0.960315	0.833258
1	-3.397061	-1.652179	-0.855934
1	-1.867082	-0.299673	2.212554
1	-0.220173	-0.713500	1.778813
1	-1.791071	1.817677	1.155765
1	-0.257678	1.639789	2.003682
1	2.073241	-2.645169	-0.208522
1	1.152337	-1.838889	1.049751
1	3.047301	1.424159	0.676680
1	1.768562	0.654204	1.613979
1	3.190277	-0.523270	-0.855089
1	3.497699	-0.977075	0.817614
6	-0.956880	2.204558	-1.227570
1	-1.314485	3.192696	-0.905009
1	-0.415444	2.324334	-2.169121
1	-1.861773	1.605954	-1.406186

Electronic energy = -467.801114  
 Sum of electronic and thermal Energies= -467.517793  
 Sum of electronic and thermal Enthalpies = -467.516849  
 Sum of electronic and thermal Free Energies= -467.567489  
 S\*\*2 = 0.7620

-----  
 9\*+ - B3LYP/6-31G\*  
 -----

1,2  
 6 0.020380 -0.368284 1.316074  
 6 1.517080 -0.233776 0.991974  
 6 -2.103471 0.285377 0.003391  
 6 -0.628453 -0.002074 -0.050485  
 6 1.558083 1.027333 0.187977  
 6 -2.668674 1.233738 -0.814640  
 6 2.623802 1.880767 0.094260  
 6 0.224457 1.230903 -0.483297  
 6 -0.381151 -1.216458 -1.020099  
 6 1.940599 -1.454528 0.085633  
 6 1.125232 -1.500732 -1.210988  
 1 2.168675 -0.207760 1.870822  
 1 -0.267974 0.353323 2.090420  
 1 -0.245842 -1.368771 1.667286  
 1 2.561692 2.815706 -0.456299  
 1 3.575730 1.644878 0.562412  
 1 -0.228406 2.166349 -0.106275  
 1 0.313081 1.353894 -1.569817  
 1 -3.732964 1.445480 -0.770898  
 1 -2.091614 1.796666 -1.540407  
 1 1.777166 -2.352503 0.693545  
 1 3.010493 -1.397059 -0.135369  
 1 -0.883376 -2.097705 -0.604545  
 1 -0.841274 -1.014195 -1.993070  
 1 1.231275 -2.490572 -1.671966  
 1 1.540680 -0.784938 -1.930084  
 6 -2.958311 -0.501475 0.945434  
 1 -2.675573 -0.287961 1.987258  
 1 -4.020374 -0.278686 0.824682  
 1 -2.808833 -1.580896 0.810908

Electronic energy = -467.787174  
 Sum of electronic and zero-point Energies= -467.517491  
 Sum of electronic and thermal Enthalpies = -467.504870  
 Sum of electronic and thermal Free Energies= -467.554712  
 S\*\*2 = 0.7581

-----  
 TS - 2a\*+ --> 7a\*+ - B3LYP/6-31G\*  
 -----

1,2  
 6 0.660299 -0.354040 -1.253814  
 6 -0.879120 0.052338 -0.925953  
 6 -0.077181 1.184532 0.035801  
 6 1.327664 0.818187 -0.496848  
 6 -1.752533 -0.664899 -0.029136  
 6 -0.472550 0.735277 1.474896  
 6 -2.939942 -1.219412 -0.439849  
 6 -1.264134 -0.594975 1.397263  
 6 2.415366 0.219301 0.406038

6	1.232225	-1.656036	-0.656405
6	2.042509	-1.267263	0.602616
1	-1.361958	0.405893	-1.837549
1	0.718622	-0.288142	-2.343467
1	1.716383	1.609579	-1.140883
1	-3.573529	-1.775485	0.246021
1	-3.275745	-1.140008	-1.470199
1	-2.092930	-0.625732	2.110159
1	-0.635258	-1.466203	1.618995
1	-1.110942	1.516476	1.900617
1	0.405995	0.656942	2.119047
1	1.907152	-2.049092	-1.429366
1	0.480720	-2.430584	-0.479569
1	3.371255	0.299874	-0.122906
1	2.538936	0.760240	1.350116
1	2.929671	-1.897372	0.712041
1	1.455042	-1.410134	1.513814
6	-0.547569	2.580384	-0.354108
1	-1.614376	2.719245	-0.155197
1	0.019459	3.303393	0.250870
1	-0.348706	2.810741	-1.405553

Electronic energy = -467.778210  
Sum of electronic and zero-point Energies= -467.507961  
Sum of electronic and thermal Enthalpies = -467.496169  
Sum of electronic and thermal Free Energies= -467.544042  
S\*\*2 = 0.7635

Low frequencies --- -239.9659 -23.5306 -14.3195 -0.0011 -0.0008 -0.0004  
Low frequencies --- 7.9636 80.0817 141.4741

-----  
TS - 7a\*+ --> 7b\*+ - B3LYP/6-31G\*  
-----

1,2

6	2.533236	-0.874525	0.743644
6	1.720060	0.380318	1.167575
6	1.034388	0.885015	-0.121437
6	0.819807	-0.399658	-1.031341
6	2.035979	-1.311137	-0.661331
6	-0.512211	-1.098104	-0.946377
6	-1.554536	-1.093595	-0.005404
6	-1.539082	-0.228158	1.238927
6	-1.294979	1.280332	0.947272
6	-0.278324	1.551759	-0.097104
6	-0.572698	2.563529	-1.134769
6	-2.629039	-1.940458	-0.208944
1	-0.640618	-1.812187	-1.759939
1	0.911212	-0.063512	-2.070468
1	1.740176	1.513137	-0.677165
1	-3.479727	-1.953819	0.464782
1	-2.655043	-2.631214	-1.046347
1	-2.499490	-0.302235	1.755071
1	-0.791484	-0.611652	1.938154
1	-2.236485	1.769582	0.682263
1	-0.940417	1.757669	1.877595
1	2.822202	-1.175159	-1.409735
1	1.743619	-2.365518	-0.689003
1	2.356433	1.167229	1.583375

1	0.998225	0.125274	1.944636
1	3.601592	-0.645516	0.705671
1	2.412876	-1.673142	1.480467
1	-1.627321	2.575673	-1.426181
1	-0.366846	3.554450	-0.685749
1	0.075491	2.479037	-2.011697

Electronic energy = -467.780370  
 Sum of electronic and zero-point Energies= -467.509661  
 Sum of electronic and thermal Enthalpies = -467.497428  
 Sum of electronic and thermal Free Energies= -467.547441  
 S\*\*2 = 0.7708

Low frequencies --- -123.9466 -0.0006 0.0003 0.0006 6.3232 7.2176  
 Low frequencies --- 10.9914 42.6833 76.7348

-----  
 TS - 7b\*+ --> 8b\*+ - B3LYP/6-31G\*  
 -----

1,2			
6	0.549067	-0.865097	-0.961025
6	-0.910195	-1.114663	-1.007150
6	0.112054	1.601280	-0.096965
6	1.115501	0.614774	-0.442194
6	-1.825248	-0.822058	0.016717
6	-0.914611	1.369865	0.954178
6	-3.160530	-1.149727	-0.122387
6	-1.343056	-0.085998	1.257045
6	2.079755	0.253470	0.751817
6	1.339589	-1.881512	-0.068165
6	2.592883	-1.145633	0.396649
1	-1.297919	-1.572025	-1.914536
1	0.937880	-0.931517	-1.980857
1	1.729735	0.997507	-1.261103
1	-3.885787	-0.940450	0.657459
1	-3.527360	-1.642682	-1.017639
1	-2.146341	-0.035050	1.997296
1	-0.523329	-0.630108	1.735446
1	-1.791476	1.988307	0.723066
1	-0.498545	1.824970	1.874325
1	1.549635	-2.782634	-0.652268
1	0.730974	-2.190060	0.787997
1	2.865329	1.009706	0.833670
1	1.536309	0.232470	1.701173
1	3.333187	-1.084874	-0.409732
1	3.073816	-1.627147	1.253862
6	0.030791	2.867424	-0.854441
1	0.994179	3.191380	-1.257456
1	-0.626097	2.666794	-1.724853
1	-0.450184	3.672661	-0.290321

Electronic energy = -467.784652  
 Sum of electronic and zero-point Energies= -467.514744  
 Sum of electronic and thermal Enthalpies = -467.502804  
 Sum of electronic and thermal Free Energies= -467.551086  
 S\*\*2 = 0.7784

Low frequencies --- -39.4312 -13.4931 -0.0007 -0.0004 0.0007 3.8981  
 Low frequencies --- 10.8224 82.6057 136.2363

## Compound 3

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3a\*+ - B3LYP/6-31G\*

-----

1,2

6	-0.609052	0.604466	0.753316
6	0.506000	0.424904	-0.645993
6	-0.928053	-0.886616	0.542703
6	0.130303	-1.064988	-0.597449
6	1.831105	0.604595	-0.114068
6	2.313164	-0.693165	0.491590
6	1.441697	-1.776763	-0.191950
6	2.532854	1.794977	-0.172836
6	-1.813269	1.428315	0.345372
6	-2.651898	0.489097	-0.541120
6	-2.398343	-0.905031	0.072347
1	0.140149	1.103337	-1.415441
1	-0.308293	-1.459786	-1.517620
1	-0.046033	0.935527	1.624330
1	-0.733939	-1.530932	1.405053
1	3.560119	1.863208	0.174045
1	2.087348	2.694023	-0.589978
1	2.153702	-0.663479	1.580461
1	3.388561	-0.838284	0.347876
1	1.944237	-2.134102	-1.097397
1	1.266433	-2.644926	0.448775
1	-2.597374	-1.726975	-0.622001
1	-3.044257	-1.048838	0.946593
1	-2.308352	0.531868	-1.582438
1	-3.710432	0.760446	-0.546168
1	-1.571456	2.400843	-0.095151
1	-2.347462	1.639321	1.287591

Electronic energy = -428.473271

Sum of electronic and zero-point Energies= -428.230395

Sum of electronic and thermal Enthalpies = -428.219558

Sum of electronic and thermal Free Energies= -428.265874

S\*\*2 = 0.7649

-----

3b\*+ - B3LYP/6-31G\*

-----

1,2

6	0.620329	0.609036	-0.537125
6	-0.584426	0.341389	0.747733
6	0.926612	-0.895539	-0.345615
6	-0.272899	-1.159656	0.610424
6	-1.845293	0.634123	0.115336
6	-2.330382	-0.578493	-0.639874
6	-1.550021	-1.765460	-0.019468
6	-2.486524	1.860755	0.199297
6	1.825712	1.447587	-0.124378
6	2.981012	0.413043	-0.182349
6	2.336359	-0.906888	0.287207
1	-0.263553	0.932722	1.603733
1	0.020570	-1.664157	1.534015
1	0.115961	0.918134	-1.451641
1	0.880608	-1.466162	-1.280353
1	-3.478243	2.009145	-0.218987

1	-2.027972	2.704014	0.708591
1	-2.109442	-0.446985	-1.710396
1	-3.418664	-0.685632	-0.573941
1	-2.153330	-2.226177	0.769322
1	-1.323677	-2.545652	-0.751144
1	2.261264	-0.919864	1.381855
1	2.908761	-1.790606	-0.007847
1	3.831503	0.718142	0.433518
1	3.337376	0.316736	-1.214253
1	1.730334	1.838853	0.895410
1	1.965636	2.308109	-0.785011

Electronic energy = -428.467995  
Sum of electronic and zero-point Energies= -428.225215  
Sum of electronic and thermal Enthalpies = -428.214186  
Sum of electronic and thermal Free Energies= -428.261231  
S\*\*2 = 0.7637

-----  
10\*+ - B3LYP/6-31G\*  
-----

1,2			
6	0.629724	-0.613712	0.534049
6	-0.586984	-0.802662	-0.377631
6	0.993398	0.904325	0.214238
6	-0.206392	1.070089	-0.667714
6	-1.955917	-0.617903	0.053869
6	-2.158473	0.681452	0.808150
6	-1.470695	1.713255	-0.120845
6	-2.944555	-1.453111	-0.363084
6	1.890783	-1.427540	0.158825
6	3.037918	-0.401678	0.177293
6	2.398744	0.866412	-0.417262
1	-0.434923	-1.447099	-1.244228
1	-0.032854	1.096724	-1.746187
1	0.332518	-0.714875	1.583595
1	0.945396	1.526743	1.112424
1	-3.968203	-1.334454	-0.018219
1	-2.741319	-2.294055	-1.020785
1	-1.677422	0.647690	1.794407
1	-3.213183	0.915745	0.967743
1	-2.140500	1.963814	-0.949040
1	-1.214325	2.641975	0.403363
1	2.324995	0.775239	-1.508622
1	2.960663	1.780380	-0.203528
1	3.912152	-0.739303	-0.386192
1	3.364256	-0.213978	1.207161
1	1.784344	-1.856488	-0.844955
1	2.033100	-2.261621	0.853726

Electronic energy = -428.462313  
Sum of electronic and zero-point Energies= -428.219393  
Sum of electronic and thermal Enthalpies = -428.208349  
Sum of electronic and thermal Free Energies= -428.255185  
S\*\*2 = 0.7619

-----  
11\*+ - B3LYP/6-31G\*  
-----

1,2

6	-2.113754	0.837355	0.529130
6	1.511935	-0.108804	1.067072
6	-1.016889	-0.029958	0.917222
6	0.419228	0.836730	0.864377
6	2.312473	-0.270807	-0.074186
6	1.793197	0.623046	-1.190693
6	0.741382	1.523533	-0.490491
6	3.415239	-1.088668	-0.113052
6	-2.936628	0.270738	-0.560245
6	-2.575906	-1.232847	-0.544865
6	-1.122750	-1.263437	-0.018074
1	1.665805	-0.659805	1.991896
1	0.293453	1.540515	1.693018
1	-2.291323	1.812864	0.977485
1	-1.067725	-0.285376	1.984461
1	4.044912	-1.158912	-0.995155
1	3.707407	-1.680571	0.749661
1	1.348760	0.014871	-1.987298
1	2.595915	1.205901	-1.651825
1	1.168927	2.509235	-0.282769
1	-0.145779	1.687268	-1.108467
1	-0.422558	-1.158699	-0.853810
1	-0.876390	-2.196814	0.494388
1	-2.678313	-1.704161	-1.525101
1	-3.244314	-1.757905	0.145372
1	-2.661025	0.751842	-1.518958
1	-4.002923	0.498463	-0.430067

Electronic energy = -428.463292  
Sum of electronic and zero-point Energies= -428.222284  
Sum of electronic and thermal Enthalpies = -428.210549  
Sum of electronic and thermal Free Energies= -428.259638  
S\*\*2 = 0.7831

-----  
12\*+ - B3LYP/6-31G\*  
-----

1,2

6	-3.110230	0.646079	-0.239297
6	-2.984157	-0.863840	-0.573540
6	-1.766642	-1.302499	0.185940
6	-1.353379	-0.351591	1.067128
6	-2.242061	0.858161	1.028921
6	0.685079	0.104751	-1.106522
6	1.566198	-0.870385	-0.682959
6	2.611812	-0.290336	0.096576
6	2.364388	1.200902	0.222365
6	1.124517	1.464434	-0.666324
6	3.667190	-0.992161	0.624481
1	3.759006	-2.064401	0.478032
1	4.447409	-0.501777	1.198961
1	3.237161	1.779152	-0.098923
1	2.180836	1.471720	1.269265
1	0.325623	2.015574	-0.153874
1	1.367919	2.068866	-1.553426
1	1.497583	-1.926289	-0.922844
1	-0.551986	-0.484793	1.788154



1	-2.922940	-1.074266	-1.649098
1	-3.852433	-1.439486	-0.214391
1	-2.713019	1.244066	-1.067194
1	-4.146814	0.956515	-0.092060
1	-1.685986	1.806020	1.025519
1	-2.849383	0.886059	1.947787
1	-0.137490	-0.063947	-1.791947
1	-1.331774	-2.294098	0.095433

Electronic energy = -428.478108  
 Sum of electronic and zero-point Energies= -428.239212  
 Sum of electronic and thermal Enthalpies = -428.226099  
 Sum of electronic and thermal Free Energies= -428.281148  
 S\*\*2 = 0.7665

-----  
 TS - 3a\*+ --> 3b\*+ - B3LYP/6-31G\*  
 -----

1,2			
6	-0.616929	0.495282	0.708285
6	0.532180	0.321729	-0.715748
6	-0.960327	-0.962818	0.389192
6	0.256881	-1.178966	-0.561772
6	1.820399	0.656175	-0.179996
6	2.382440	-0.532851	0.566135
6	1.556844	-1.747329	0.063654
6	2.424371	1.890337	-0.332106
6	-1.781800	1.417931	0.438414
6	-2.912263	0.528480	-0.147317
6	-2.336453	-0.907303	-0.323448
1	0.094477	0.918174	-1.514471
1	-0.023565	-1.693466	-1.484746
1	0.001441	0.714344	1.576946
1	-0.952061	-1.620479	1.266106
1	3.430231	2.076943	0.033522
1	1.922288	2.706291	-0.844634
1	2.270265	-0.369657	1.648289
1	3.458207	-0.642203	0.392645
1	2.117908	-2.276107	-0.712976
1	1.352789	-2.469333	0.858874
1	-2.221859	-1.148161	-1.385513
1	-3.009952	-1.660937	0.093012
1	-3.284000	0.924906	-1.095521
1	-3.761123	0.520771	0.541678
1	-1.516726	2.265954	-0.203880
1	-2.070374	1.868961	1.398906

Electronic energy = -428.465687  
 Sum of electronic and zero-point Energies= -428.223234  
 Sum of electronic and thermal Enthalpies = -428.212736  
 Sum of electronic and thermal Free Energies= -428.258880  
 S\*\*2 = 0.7661

Low frequencies --- -143.3210 -17.1337 -0.0006 -0.0004 0.0006 5.4949  
 Low frequencies --- 15.5032 49.4510 99.0926

-----  
TS - 10\*+ --> 3b\*+ - B3LYP/6-31G\*  
-----

1,2  
6 0.624358 -0.570409 0.540878  
6 -0.610677 -0.667577 -0.461336  
6 1.030453 0.910667 0.249753  
6 -0.186535 0.992753 -0.655256  
6 -1.971462 -0.586710 0.023581  
6 -2.209250 0.721487 0.747263  
6 -1.434284 1.727307 -0.134257  
6 -2.924772 -1.522743 -0.285646  
6 1.838730 -1.442620 0.147744  
6 3.028763 -0.463500 0.182261  
6 2.441505 0.849768 -0.369661  
1 -0.441503 -1.347557 -1.295516  
1 0.042387 1.097705 -1.721779  
1 0.248714 -0.710737 1.559659  
1 0.974385 1.568469 1.119766  
1 -3.930608 -1.462872 0.121314  
1 -2.698967 -2.370346 -0.927220  
1 -1.799334 0.673021 1.767007  
1 -3.269212 0.969351 0.839633  
1 -2.055186 2.018134 -0.988752  
1 -1.152835 2.638060 0.403247  
1 2.378906 0.804178 -1.464646  
1 3.039940 1.728722 -0.115650  
1 3.882200 -0.826805 -0.397300  
1 3.369483 -0.321380 1.214654  
1 1.717735 -1.856628 -0.860033  
1 1.932917 -2.291852 0.833671

Electronic energy = -428.461858  
Sum of electronic and zero-point Energies= -428.219942  
Sum of electronic and thermal Enthalpies = -428.209518  
Sum of electronic and thermal Free Energies= -428.255039  
S\*\*2 = 0.7628

Low frequencies --- -201.5055 -3.0100 -0.0009 -0.0007 -0.0001 7.2372  
Low frequencies --- 10.1759 56.7657 156.1001

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TS - 3b\*+ --> 11\*+ - B3LYP/6-31G\*  
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1,2  
6 -1.632122 1.060220 -0.339834  
6 1.313720 -0.531122 0.964432  
6 -1.081029 0.406958 0.831445  
6 0.563679 0.710938 1.141913  
6 2.049250 -0.540376 -0.234832  
6 1.827765 0.784549 -0.951286  
6 1.258188 1.690637 0.163514  
6 2.853558 -1.580446 -0.628604  
6 -2.441558 0.152547 -1.181336  
6 -2.761033 -1.025027 -0.231331  
6 -1.534368 -1.077888 0.702570  
1 1.292511 -1.359760 1.666617  
1 0.559520 1.060103 2.175547  
1 -1.519289 2.120976 -0.546381  
1 -1.515533 0.887262 1.720428

1	3.443435	-1.535138	-1.539323
1	2.941465	-2.481556	-0.028203
1	1.106055	0.650698	-1.769654
1	2.741849	1.184532	-1.398560
1	2.081502	2.171903	0.702061
1	0.614103	2.489774	-0.208664
1	-0.745629	-1.670399	0.226687
1	-1.749841	-1.535822	1.671192
1	-2.927665	-1.966025	-0.760934
1	-3.670278	-0.796356	0.334685
1	-1.837308	-0.184100	-2.046183
1	-3.311181	0.657962	-1.619214

Electronic energy = -428.456338  
Sum of electronic and zero-point Energies= -428.215361  
Sum of electronic and thermal Enthalpies = -428.204569  
Sum of electronic and thermal Free Energies= -428.251145  
S\*\*2 = 0.7808

Low frequencies --- -60.2585 -18.6310 -8.8823 -4.9540 -0.0003 -0.0002  
Low frequencies --- 0.0004 63.3511 101.5906

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TS - 11\*+ --> 12\*+ - B3LYP/6-31G\*  
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1,2

6	2.124164	-0.783371	0.600633
6	-1.520630	-0.045675	1.084073
6	1.069117	0.068551	1.027585
6	-0.438856	-0.956596	0.813439
6	-2.270132	0.253186	-0.069915
6	-1.705619	-0.521721	-1.251728
6	-0.680689	-1.492896	-0.609258
6	-3.366672	1.079181	-0.074005
6	2.818389	-0.282206	-0.607816
6	2.436256	1.217112	-0.667290
6	1.127700	1.344086	0.162524
1	-1.715896	0.389229	2.060663
1	-0.226177	-1.699347	1.582089
1	2.366451	-1.727905	1.083484
1	0.965149	0.194201	2.106862
1	-3.954139	1.245188	-0.972064
1	-3.694511	1.583111	0.830597
1	-1.230540	0.160524	-1.966136
1	-2.489409	-1.052928	-1.799757
1	-1.112172	-2.496031	-0.518266
1	0.230361	-1.599126	-1.202847
1	0.253077	1.418474	-0.489833
1	1.124396	2.241275	0.787730
1	2.315815	1.576535	-1.691769
1	3.232662	1.809679	-0.207949
1	2.478363	-0.846643	-1.496139
1	3.898399	-0.474139	-0.556124

Electronic energy = -428.462755  
Sum of electronic and zero-point Energies= -428.222312  
Sum of electronic and thermal Enthalpies = -428.210863  
Sum of electronic and thermal Free Energies= -428.259561  
S\*\*2 = 0.7926  
Low frequencies --- -158.8517 -17.3718 -7.0439 -0.0006 0.0003 0.0005  
Low frequencies --- 6.3161 47.4566 73.7429